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Original Research

Analysis of retarding effect on α to γ transformation in Fe–C alloy by addition of dispersed particles

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Abstract

The effects of dispersed second phase particles on α-ferrite (α) to austenite (γ) transformation at 1140 K in Fe–C alloy were studied by means of phase field simulation. According to the simulated results, it was found that the particle could retard the migration of α/γ interface. Importantly, both the morphology of particles and the interfacial energy of particle/matrix (α or γ) interface affect the magnitude of the retarding effect. More specifically, the particles with smaller aspect ratio bring stronger retarding force, and when the interfacial energy of particle/γ interface is larger than that of particle/α interface, the retarding effect also becomes significant. These phenomena could be explained from the viewpoint of change in the total amount of the interfacial energy of the simulation system.

Keywords: α/γ Interface; Retarding effect; Particle morphology; Interfacial energy

1. Introduction

Before applying the hot forming processes such as hot rolling, forging and extrusion, the carbon steel is usually reheated above the eutectoid temperature from room temperature, during which the reverse transformation to austenite (γ) from α-ferrite (α), pearlite or martensite structures takes place inevitably. The reverse transformation has particular importance for the subsequent plastic deformation and cooling process, since the condition of reversely transformed γ significantly affects the final microstructures and mechanical properties [1–4].

In recent years, many researchers have transferred their attention from the austenite decomposition during cooling to the reverse transformation during reheating. Rudnizki [5] simulated the microstructure evolution during the formation of γ from the mixture of α and pearlite by means of the phase field method. Basabe [6] investigated the dynamic reverse transformation behavior of low carbon steel under different strains, strain rates and temperatures. Li [7] studied the effects of alloying elements on the reversion kinetics from pearlite to austenite, and proposed that the addition of different alloying elements can either accelerate or retard the kinetics. Kajihara [8] performed numerical analysis on the migration behavior of α/γ interface during isothermal carburization of Fe–C alloy. The migration distance shows parabolic relationship with the transformation time, which supports the carbon diffusion controlled mechanism. Schmidt [9] compared the kinetics of α/γ interface obtained from the numerical models and high temperature confocal scanning laser microscope. Son [10] compared the behavior of reverse transformation from ultrafine grains and coarse grains in low carbon steel.

From the above literature, it should be noticed that these early efforts mainly focused on the effects of initial microstructures and alloying elements on the kinetics of reverse transformation, while little has been addressed the retarding effect of second phase particles. The reverse transformation is a process of nucleation and growth of γ phase. It is considered that if the γ growth could be retarded, there will be more positions and time for nucleation, and

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thus the γ grains after reverse transformation could be effectively refined [11]. On the other hand, it is well known that the second phase particles could strongly retard the grain growth, which is called Zener pinning [12–17]. Based on this point, the experimental work was carried out in our previous work to study the effects of insoluble ZrO_2 and TiO_2 particles on the kinetics of α to γ transformation recently, and it was indeed found that these particles could also retard the migration of α/γ interface [18], and the retarding effect becomes noticeable for particles with higher volume fraction or smaller size.

However, there are some other factors that might influence the magnitude of the retarding effect, such as the particle morphology and the interfacial energy of particle/matrix interface, which are difficult to be clarified by performing experiments. Thus, in this paper, the isothermal α to γ transformation in Fe–C alloy was simulated by means of the phase field methods, which have been proved to be effective on providing qualitative evidence [18,19]. Importantly, the effects of particle morphology (circular and elliptical) and the interfacial energy of particle/matrix (α or γ) interface were investigated. The main objective of the present study is to study the retarding effect of particle on α to γ transformation.

2. Phase field modeling

In recent decade, the phase field method has become a powerful tool to describe a variety of microstructure evolution. The diffused interface in phase field method allows us to describe the complex morphology of the microstructure without explicitly tracking the position of the interface. In the present study, the phase field model proposed by Steinbach and Pezzola [20,21] was utilized to investigate isothermal α to γ transformation in Fe–C alloy including dispersed particles. The detailed information of the modeling is summarized below.

2.1. Phase field variables

The coexisting α, γ phases and insolvable particles are distinguished by the order parameters of ϕ_i, where the subscript i specifies the types of different phases. i and p represent α or γ phase and insoluble particles, respectively. More specifically, $\phi_\alpha=1$ and $\phi_\gamma=\phi_p=0$ in α phase, $\phi_\gamma=1$ and $\phi_\alpha=\phi_p=0$ in γ phase, $\phi_p=1$ and $\phi_\alpha=\phi_\gamma=0$ in particle region. ϕ_i varies from 0 to 1 smoothly across the thickness of phase interface. The carbon diffusion was coupled in this model and the carbon concentration, c, is given by $c=\sum_{i=1}^{n}\phi_i c_i$, where c_i is the carbon concentration associated with i phase.

2.2. Governing equation

The time evolution of the order parameter is described by the following equation:

$$\frac{\partial\varphi_i}{\partial t}=-\frac{2}{N}\sum_{j\neq i}^{n}s_{ij}M_{ij}\left[\frac{\delta F}{\delta\varphi_i}-\frac{\delta F}{\delta\varphi_j}\right] \tag{1}$$

where t is the transformation time, N is the number of coexisting phases at a given spatial point, M_{ij} is the mobility of i/j interface, F is the free energy functional of the system, s_{ij} takes 1 when i and j phases coexist and it takes 0 otherwise. Then, the next step is the derivation of the free energy functional F. The free energy functional of a system of volume V is defined as:

$$F=\int_V\left[f^P+f^T+\lambda_L\left(\sum_i\varphi_i-1\right)\right]dV \tag{2}$$

where f^P is the double well potential, f^T is the thermodynamic potential and λ_L is the Lagrange multiplier. Thus, the functional derivation in Eq. (1) can be written as:

$$\frac{\delta F}{\delta\phi_i}=\sum_{j\neq i}^{n}\left[\frac{\varepsilon_{ij}^2}{2}\nabla^2\phi_j+\omega_{ij}\phi_j\right]+\left[f^i(c_i)+\sum_j^n\phi_j f_{c_j}^j(c_j)\frac{\partial c_j}{\partial\phi_i}\right]-\lambda_L \tag{3}$$

where ε_{ij} is the gradient energy coefficient and ω_{ij} is the height of the double well potential, $f^i(c_i)$ is the free energy density of i phase with composition c_i. Moreover, when i and j phases are in equilibrium condition, the following relationship is held:

$$\frac{\delta F}{\delta\varphi_i}-\frac{\delta F}{\delta\varphi_j}=\left\{\sum_{j\neq i}^{n}\left[\frac{\varepsilon_{ij}^2}{2}\nabla^2\varphi_j+\omega_{ij}\varphi_j\right]-\sum_{j\neq i}^{n}\left[\frac{\varepsilon_{ij}^2}{2}\nabla^2\varphi_i+\omega_{ij}\varphi_i\right]\right\}+(f_i^c-f_j^c)-(c_i f_c-c_j f_c) \tag{4}$$

where f_c is the chemical potential. The condition of the equal chemical potential between the coexisting phases was introduced here [22]. In dilute alloy system, the following relation can be used:

$$\left(f_i^c-f_j^c\right)-\left(c_i f_c-c_j f_c\right)\approx-\frac{RT}{V_m}\left\{\left(c_i-c_j\right)-\left(c_i^{e,j}-c_j^{e,i}\right)\right\} \tag{5}$$

where R is the gas constant, T is the temperature and V_m is molar volume. $c_i^{e,j}$ represents the carbon concentration of i phase in equilibrium with j phase. Based on the above discussion, the final form of the evolution equation for order parameter ϕ_i is given as:

$$\frac{\partial\varphi_i}{\partial t}=-\frac{2}{N}\sum_{j\neq i}^{n}s_{ij}M_{ij}\left\{\begin{array}{c}\sum_{j\neq i}^{n}\left[\frac{\varepsilon_{ij}^2}{2}\nabla^2\varphi_j+\omega_{ij}\varphi_j\right]-\sum_{i\neq j}^{n}\left[\frac{\varepsilon_{ij}^2}{2}\nabla^2\varphi_i+\omega_{ij}\varphi_i\right]\\+\frac{RT}{V_m}\left[(c_i^{e,j}-c_j^{e,i})-(c_i-c_j)\right]\end{array}\right\} \tag{6}$$

The parameters of ε_{ij} and ω_{ij} could be calculated according to the following expressions:

$$\varepsilon_{ij}=\frac{2}{\pi}\sqrt{2\sigma_{ij}W} \tag{7}$$

$$\omega_{ij}=\frac{4\sigma_{ij}}{W} \tag{8}$$

where σ_{ij} is the interfacial energy between i and j phases, W is the interface thickness. The mobility, M_{ij} was assumed as follows [23]: